

2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine
368441-96-7 | DTXSID50364048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 319 °C

Global applicability domain: Inside

Local applicability domain index: 4.23e-01

Confidence level: 5.23e-01

Nearest Neighbors from the Training Set

Image not found

2-Methyl-5-nitro-1H-isoindole-
1,3(2H)-dione

Measured: 361

Predicted: 323

Image not found

Acibenzolar-S-methyl

Measured: 267

Predicted: 295

Image not found

1H-Pyrazole, 3,5-dimethyl-1-
phenyl-

Measured: 273

Predicted: 287

Image not found

Chlorothalonil

Measured: 350

Predicted: 319